CHARGE NUMBER: 2505

PROJECT TITLE: Identification, Characterization and Synthesis

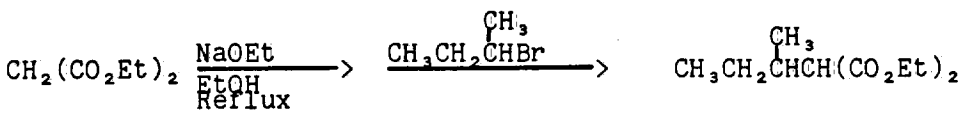
PROJECT LEADER: Roger A. Comes

PERIOD COVERED: July-August, 1984

DATE OF REPORT: August 24, 1984

1. Acid release

In anticipation of future needs and projected large scale requirements in the Oriental replacement program, several 0.2mole scale reactions to prepare diethyl sec. butylmalonate were performed as follows:



The diester is the precursor to the diacid (CR-2403) and its disodium salt (CR-2409) both of which generate β-methyl valeric acid under normal smoking conditions.

Production quantities of these materials should be readily obtainable through a contract vendor. Laboratory scale reactions have generated an inventory of 1.5kg of CR-2409. A procedure for quantitation of β-methyl valeric acid in smoke has been developed by Project Number 1740.

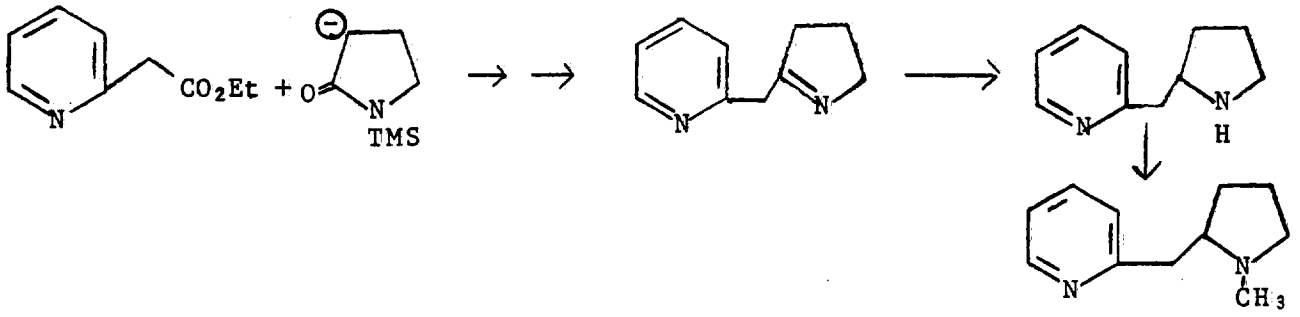
2. GC/MS Support

Multiple (15) samples were analyzed by GC/MS in support of projects within the Chemical Research Division. Additionally, two samples related to a customer complaint were run as requested. A mixture of tobacco alkaloids (approx. 5ng each) was used to evaluate the new "heart cutting" gas chromatograph with excellent results obtained. Modifications are in progress to allow pyrolyses/GC and then attachment to the Finnigan mass spec. will finalize the installation.

3. Organic Synthesis

a) A sample of N'-nitroso nornicotine was prepared at the request of Project 6908.

b) A new nicotine analog was prepared as shown:



Interest in this compound comes from the N,N' distance and similarity to nicotine with three carbon atoms intervening between the two nitrogen atoms.

c) Additional experimental work was carried out on the homo and bis homo nicotine analogs for inclusion in proposed publications.

4. Computer support

a) Additional research has been conducted into a laboratory computer system for the Chemical Research Division.

b) Miscellaneous computer applications were addressed. These included: establishment of an inventory file of all capillary GC columns on hand in the division; assistance to the division secretary and divisional personnel in computer familiarization and word processing capabilities; and connection of a liquid scintillation counter to the Perkin-Elmer 3600 computer.

5. Reports

Three special reports issued during this period.

a) "Determination of the Decomposition of a Sucrose Mono-Ester of 3-Methylvaleric Acid in Cigarettes" by D. Ingraham, July 20, 1984, Acc.#84-228.

b) "A Review of the Flavor Release Technology Developed at Philip Morris" by K. Podraza, July 27, 1984, Acc.#84-231.

c) "Data Processing of Signals from Radiochromatography Flow Proportional Counters - Part 2" by D. Ingraham, July 27, 1984, Acc. #84-232.

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